

MULTI-STAGE INFLUENCE FUNCTION

Anonymous authors

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ABSTRACT

Multi-stage training and knowledge transfer from a large-scale pretrain task to various finetune end tasks have revolutionized natural language processing (NLP) and computer vision (CV), with state-of-the-art performances constantly being improved. In this paper, we develop a multi-stage influence function score to track predictions from a finetune model all the way back to the pretrain data. With this score, we can identify the pretrain examples in the pretrain task that contribute most to a prediction in the finetune task. The proposed multi-stage influence function generalizes the original influence function for a single model in Koh & Liang (2017), thereby enabling influence computation through both pretrain and finetune models. We study two different scenarios with the pretrain embeddings fixed or updated in the finetune tasks. We test our proposed method in various experiments to show its effectiveness and potential applications.

1 INTRODUCTION

Multi-stage training has become increasingly important and has achieved state-of-the-art results in many tasks. In NLP applications, it is now a common practice to first learn word embeddings (e.g., word2vec (Mikolov et al., 2013), GloVe (Pennington et al., 2014)) or contextual representations (e.g., ELMo (Peters et al., 2018), BERT (Devlin et al., 2018)) from a large unsupervised corpus, and then refine or finetune the model on supervised end tasks. In computer vision applications, it is common to use a pretrained CNN as a feature extractor and only finetune top-layer networks through training on the end task. Also, it has been demonstrated that pretraining ResNet (He et al., 2016) with large hashtag data can greatly benefit many end tasks (Mahajan et al., 2018). Intuitively, the successes of these multi-stage learning paradigms are due to knowledge transfer from pretrain tasks to the end task. However, current approaches using multi-stage learning are usually based on trial-and-error and many fundamental questions remain unanswered. For example, which part of the pretrain data/task contributes most to the end task? How can one detect “false transfer” where some pretrain data/task could be harmful for the end task? If a testing point is wrongly predicted by the finetune model, can we trace back to the problematic examples in the pretrain data? Answering these questions requires a quantitative measurement of how the data and loss function in the pretrain stage influence the end model, which has not been studied in the past and will be the main focus of this paper.

To find the most influential training data responsible for a model’s prediction, the influence function was first introduced by Cook & Weisberg (1980) from a robust statistics point of view. Recently, as large-scale applications become more challenging for influence function computation, Koh & Liang (2017) proposed to use a first-order approximation to measure the effect of removing one training point on the model’s prediction, to overcome computational challenges. More broadly, there are many works using influence functions to investigate the impact of training data on models in various machine learning applications, such as tracing back the origins of bias in the word embeddings generated by GloVe (Brunet et al., 2019), and understanding and mitigating disparate impact to improve model fairness (Wang et al., 2019). However, all of the existing influence score computation algorithms study the case of single-stage training – where there is only one model with one set of training/prediction data in the training process. To the best of our knowledge, the influence of pretrain data on a subsequent finetune task and model has not been studied, and it is nontrivial to apply the original influence function in (Koh & Liang, 2017) to this scenario.

In this work, we derive the influence function from pretrain data to the end task in multi-stage training. Since the computation involves several expensive Hessian vector products, we also show how to

compute the influence function efficiently in large-scale problems. Based on this technique, we show that

- in real datasets and experiments across various vision and NLP tasks, predictions using the technique and actual influence for the pretrain data to the finetune model are highly correlated (Pearson’s r score to be around 0.6). This shows the effectiveness of our proposed technique for computing the influence scores in multi-stage models;
- the influence for the pretrain data to the finetune model can be split into two parts: the influence of the pretrain data on the pretrain model, and influence of the pretrain data on the finetune model. Therefore the testing data from the finetune task will be impacted by changes in the pretrain data, which can be quantified using our proposed technique;
- the influence of the pretrain data on the finetune task is highly dependent on 1) the similarity of two tasks or stages, 2) and the number of training data in the finetune task. Thus our proposed technique provides a novel way to measure how the pretrain data helps or benefits the finetune data.

2 RELATED WORK

Multi-stage model training that trains models in many stages on different tasks to improve the end-task has been used widely in many machine learning areas, such as in transfer learning (Ando & Zhang, 2005) and zero-shot learning (Larochelle et al., 2008). Recently, multi-stage model training has achieved state-of-the-art performance by learning large embeddings or data representation as the pretrain step on a very large pretrain dataset, which is then followed by a finetune step with further training on the end-task. Examples include the recently proposed BERT (Devlin et al., 2018), which learns contextual embeddings on a large corpus with the pretrain tasks chosen to be predicting the masked words in a sentence and predicting whether one sentence is after another sentence. This contextual embedding is then used in finetune tasks, such as a question answering task. ELMo (Peters et al., 2018) is widely used in multi-stage model training as a sentence feature extractor to benefit the end-task. Similarly, there are some works in computer vision that train an image representation model on a large number of images as the pretrain step, and then use the resulting features to finetune another task, such as particular image classification tasks. For example, (Mahajan et al., 2018) uses ResNet in the pretrain step, and the finetune task is based on hashtag data. The rationale for this multi-stage model is that the pretrain task can learn some common or latent representation which could benefit the end task.

Another related line of research is on understanding machine learning models. One category of research is to explain predictions with respect to model variables, and trace back the contribution of variables to the prediction. For example, Oramas et al. (2019) automatically detects internal features in the set of classes in the pretrain model that are relevant to interpreting the prediction, and shows for various vision tasks that the proposed scheme can produce detailed explanations based on the features that are relevant to the targeted classes. Guo et al. (2019) aims to interpret variable-wise hidden states in an LSTM model to quantify variable importance and variable-wise temporal importance in the model.

Closely related research has sought to connect model prediction and training data, and trace back the most influential training data that are most responsible for the model prediction. Among them, the influence function (Cook & Weisberg, 1980; Koh & Liang, 2017), which aims to model the prediction changes when training data is added/removed, has been shown to be effective in many applications. There is a series of work on influence functions, including investigating the influence of a group of data on the prediction (Koh et al., 2019), using influence functions to detect bias in word embeddings (Brunet et al., 2019), and using it in preventing data poisoning attacks (Steinhardt et al., 2017), etc. All of these works only consider a single stage training procedure, and it is not straightforward to apply the existing influence functions to multi-stage models. In this paper, we propose to analyze the influence of pretrain data on predictions in the subsequent finetune model and end task.

3 ALGORITHMS

In this section, we detail the procedure of multi-stage training, show how to compute the influence score for the multi-stage training, and then discuss how to scale up the computation.

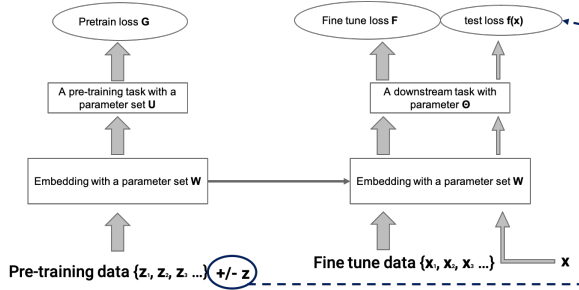


Figure 1: The setting for influence functions in multi-stage models. We consider a two-stage model, where we have a first pretrain model, and a second finetune model for a desired end task. We seek to compute the influence of the pretrain data on predictions using testing data in the finetune task.

3.1 MULTI-STAGE MODEL TRAINING

Multi-stage models, which train different models in consecutive stages, have been widely used in various ML tasks. Mathematically, let \mathcal{Z} be the training set for pretrain task with data size $|\mathcal{Z}| = m$, and \mathcal{X} be the training data for the finetune task with data size $|\mathcal{X}| = n$. In pretrain stage, we assume the parameters of the pretrain network have two parts: the parameters W that are shared with the end task, and the task-specific parameters U that will only be used in the pretrain task. Note that W could be a word embedding matrix (e.g., in word2vec) or a representation extraction network (e.g., Elmo, BERT, ResNet), while U is usually the last few layers that corresponds to the pretrain task. After training on the pretrain task, we obtain the optimal parameters W^*, U^* . The pretrain stage can be formulated as

$$\text{Pretrain Stage: } W^*, U^* = \arg \min_{W, U} \frac{1}{m} \sum_{z \in \mathcal{Z}} g(z, W, U) := \arg \min_{W, U} G(W, U), \quad (1)$$

where $g(\cdot)$ is the loss function for the pretrain task.

In the finetune stage, the network parameters are W, Θ , where W is shared with the pretrain task and Θ is the rest of the parameters specifically associated with the finetune task. We will initialize the W part by W^* . Let $f(\cdot)$ denote the finetune loss, there are two cases when finetune the end-task:

- Finetune Case 1: Fixing embedding parameters $W = W^*$, and only finetune Θ :

$$\Theta^* = \arg \min_{\Theta} \frac{1}{n} \sum_{x \in \mathcal{X}} f(x, W^*, \Theta) := \arg \min_{\Theta} F(W^*, \Theta). \quad (2)$$

- Finetune Case 2: finetune both the embedding parameters W (initialized from W^*) and Θ . Sometimes updating the embedding parameters W in the finetune stage is necessary, as the embedding parameters from the pretrain model may not be good enough for the finetune task. This corresponds to the following formulation:

$$W^{**}, \Theta^* = \arg \min_{W, \Theta} \frac{1}{n} \sum_{x \in \mathcal{X}} f(x, W, \Theta) := \arg \min_{W, \Theta} F(W, \Theta). \quad (3)$$

3.2 INFLUENCE FUNCTION FOR MULTI-STAGE MODELS

We derive the influence function for the multi-stage model to trace the influence of pretrain data on the finetune model. In Figure 1 we show the task we are interested in solving in this paper. Note that we use the same definition of influence function as (Koh & Liang, 2017) and discuss how to compute it in the multi-stage training scenario. As discussed at the end of Section 3.1, depending on whether or not we are updating the shared parameters W in the finetune stage, we will derive the influence functions under two different scenarios.

3.2.1 CASE 1: EMBEDDING PARAMETERS W ARE FIXED IN FINETUNE

To compute the influence of pretrain data on the finetune task, the main idea is to perturb one data example in the pretrain data, and study how that impacts the test data. Mathematically, if we perturb

a pretrain data example z with loss change by a small ϵ , the perturbed model can be defined as

$$\hat{W}_\epsilon, \hat{U}_\epsilon = \arg \min_{W, U} G(W, U) + \epsilon g(z, W, U). \quad (4)$$

Note that choices of ϵ can result in different effects in the loss function from the original solution in (1). For instance, if we set $\epsilon = -\frac{1}{n}$, then we are removing the training data z in the pretrain dataset.

For the finetune stage, since we consider Case 1 where the embedding parameters W are fixed in the finetune stage, the new model for the end-task or finetune task will thus be

$$\hat{\Theta}_\epsilon = \arg \min_{\Theta} F(\hat{W}_\epsilon, \Theta). \quad (5)$$

The influence function that measures the impact of a small ϵ perturbation on z to the finetune loss on a test sample x_t from finetune task is defined as

$$I_{z, x_t} := \left. \frac{\partial f(x_t, \hat{W}_\epsilon, \hat{\Theta}_\epsilon)}{\partial \epsilon} \right|_{\epsilon=0} \quad (6)$$

$$= \nabla_{\Theta} f(x_t, W^*, \Theta^*)^T \cdot I_{z, \Theta} + \nabla_W f(x_t, W^*, \Theta^*)^T \cdot I_{z, W}. \quad (7)$$

$$\text{with } I_{z, \Theta} := \left. \frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon} \right|_{\epsilon=0} \text{ and } I_{z, W} := \left. \frac{\partial \hat{W}_\epsilon}{\partial \epsilon} \right|_{\epsilon=0}, \quad (8)$$

where $I_{z, \Theta}$ measures the influence of z on the finetune task parameters Θ , and $I_{z, W}$ measures how z influences the pretrain model W . Therefore we can split the influence of z on the test sample into two pieces: one is the impact of z on the pretrain model $I_{z, W}$, and the other is the impact of z on the finetune model $I_{z, \Theta}$. It is worth mentioning that, due to linearity, if we want to estimate a set of test example influence function scores with respect to a set of pretrain examples, we can simply sum up the pair-wise influence functions, and so define

$$I_{\{z^{(i)}\}, \{x_t^{(j)}\}} := \sum_i \sum_j I_{z^{(i)}, x_t^{(j)}}. \quad (9)$$

where $\{z^{(i)}\}$ and $\{x_t^{(j)}\}$ contain a set of pretrain training data and finetune test data. Next we will derive these two influence scores $I_{z, \Theta}$ and $I_{z, W}$ (see the detailed derivations in the appendix) in Theorem 1 below.

Theorem 1. *For the two-stage training procedure in (1) and (2), we have*

$$I_{z, W} := \left. \frac{\partial \hat{W}_\epsilon}{\partial \epsilon} \right|_{\epsilon=0} = - \left[\left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \right]_W \quad (10)$$

$$I_{z, \Theta} := \left. \frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon} \right|_{\epsilon=0} = \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} \right)^{-1} \cdot \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} \right) \cdot \left[\left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \right]_W$$

where $[\cdot]_W$ means taking the W part of the vector.

By plugging (10) into (7), we finally obtain the influence score of pretrain data z on the finetune task testing point x_t , I_{z, x_t} as

$$I_{z, x_t} = \left[\frac{\partial f(x, W^*, \Theta^*)^T}{\partial \Theta} \cdot \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} \right)^{-1} \cdot \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} - \frac{\partial f(x, W^*, \Theta^*)^T}{\partial W} \right] I_{z, W} \quad (11)$$

Algorithm 1 shows how to compute the influence score in (11). The pseudocode for computing the influence function in (11) is shown in Algorithm 1.

3.2.2 CASE 2: EMBEDDING PARAMETER W IS ALSO UPDATED IN THE FINETUNE STAGE

For the second finetune stage case in (3), we will also further train the embedding parameter W from the pretrain stage. When W is also updated in the finetune stage, it is challenging to characterize the influence since the pretrain embedding W^* is only used as an initialization. In general, the final model (W^{**}, Θ^*) may be totally unrelated to W^* ; for instance, when the objective function is strongly convex, any initialization of W in (3) will converge to the same solution.

Algorithm 1: Multi-Stage Influence Score with Fixed Embedding

- 1 **Input:** pretrain and finetune models with W^* , Θ^* , and U^* ; pretrain and finetune training data \mathcal{Z} and \mathcal{X} ; test example x_t ; and a pretrain training example z ;
- 2 **Output:** Influence function value I_{z,x_t} ;
- 3 Compute finetune model’s gradients $\frac{\partial f(x_t, W^*, \Theta^*)}{\partial \Theta}$ and $\frac{\partial f(x_t, W^*, \Theta^*)}{\partial W}$;
- 4 Compute the first inverse Hessian vector product $V_{ihvp1}(x_t) := (\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2})^{-1} \frac{\partial f(x_t, W^*, \Theta^*)}{\partial \Theta}$;
- 5 Compute finetune loss’s gradient w.r.t W : $\frac{\partial f(x_t, W^*, \Theta^*)^T}{\partial W} = V_{ihvp1}^T \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} - \frac{f(x_t, W^*, \Theta^*)}{\partial W}$ and concatenate it with 0 to make it the same dimension as (W, U) ;
- 6 Compute and save the second inverse Hessian vector product $V_{ihvp2}(x_t) := [\frac{\partial f(x_t, \Theta^*, W^*)^T}{\partial W}, 0](\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2})^{-1}$;
- 7 Compute influence function score $I_{z,x_t} = V_{ihvp2}^T(x_t) \frac{\partial g(z, W^*, U^*)}{\partial (W, U)}$;

However, in practice the initialization of W will strongly influence the finetune stage in deep learning, since the finetune objective is usually highly nonconvex and initializing W with W^* will converge to a local minimum near W^* . Therefore, we propose to approximate the whole training procedure as

$$\bar{W}, \bar{U} = \arg \min_{W, U} G(W, U) \quad (12)$$

$$W^*, \Theta^* = \arg \min_{W, \Theta} \{\alpha \|W - \bar{W}\|_F^2 + F(W, \Theta)\},$$

where \bar{W}, \bar{U} are optimal for the pretrain stage, W^*, Θ^* are optimal for the finetune stage, and $0 \leq \alpha \ll 1$ is a small value. This is to characterize that in the finetune stage, we are targeting to find a solution that minimizes $F(W, \Theta)$ and is close to \bar{W} . In this way, the pretrain parameters are connected with finetune task and thus influence of pretrain data to the finetune task can be tractable. The results in our experiments show that with this approximation, the computed influence score can still reflect the real influence quite well.

Similarly we can have $\frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon}$, $\frac{\partial \hat{W}_\epsilon}{\partial \epsilon}$, and $\frac{\partial \bar{W}_\epsilon}{\partial \epsilon}$ to measure the difference between their original optimal solutions in (12) and the optimal solutions from ϵ perturbation over the pretrain data z . Similar to (7), the influence function I_{z,x_t} that measures the influence of ϵ perturbation to pretrain data z on test sample x_t ’s loss is

$$I_{z,x_t} := \frac{\partial f(x_t, \hat{W}_\epsilon, \hat{\Theta}_\epsilon)}{\partial \epsilon} \Big|_{\epsilon=0} = \frac{\partial f(x_t, W^*, \Theta^*)^T}{\partial (W, \Theta)} \begin{bmatrix} \frac{\partial \hat{W}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} \\ \frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} \end{bmatrix}. \quad (13)$$

The influence function of small perturbation of $G(W, U)$ to \bar{W}, W^*, Θ^* can be computed following the same approach in Subsection 3.2.1 by replacing \bar{W} for W^* and $[\Theta^*, W^*]$ for Θ^* in (10). This will lead to

$$\begin{aligned} \frac{\partial \bar{W}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} &= - \left[\left(\frac{\partial^2 G(\bar{W}, \bar{U})}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, \bar{W}, \bar{U})}{\partial (W, U)} \right) \right]_W \\ \begin{bmatrix} \frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} \\ \frac{\partial \hat{W}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} \end{bmatrix} &= \begin{bmatrix} \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} & \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} \\ \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} & \frac{\partial^2 F(W^*, \Theta^*)}{\partial W^2} + 2\alpha I \end{bmatrix}^{-1} \begin{bmatrix} 0 \\ -2\alpha I \end{bmatrix} \left[\left(\frac{\partial^2 G(\bar{W}, \bar{U})}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, \bar{W}, \bar{U})}{\partial (W, U)} \right) \right]_W \end{aligned} \quad (14)$$

After plugging (14) into (13), we will have the influence function I_{z,x_t} . Similarly, the algorithm for computing I_{z,x_t} for Case 2 can follow Algorithm 1 for Case 1 by replacing gradient computation.

3.3 IMPLEMENTATION DETAILS

The influence function computation for multi-stage model is presented in the previous section. As we can see in Algorithm 1 that the influence score computation involves many Hessian matrix operations, which will be very expensive and sometimes unstable for large-scale models. We used several strategies to speed up the computation and make the scores more stable.

Large Hessian Matrices A Hessian matrix H has a size of $p \times p$, where p is the number of parameters in the model. For large deep learning models with thousands or even millions of parameters, it

is almost impossible to fit a $p \times p$ Hessian into memory. Also, to invert a Hessian requires $O(p^3)$ operations. Similar to Koh & Liang (2017), we avoid explicitly computing and storing the Hessian matrix and its inverse, and instead compute product of the inverse Hessian with a vector directly. Every time we need an inverse Hessian vector product $v = H^{-1}b$, we invoke conjugate gradients (CG), which transforms the linear system problem into an quadratic optimization problem

$$H^{-1}b \equiv \arg \min_x \left\{ \frac{1}{2} x^T H x - b^T x \right\}. \quad (15)$$

In each iteration of CG, instead of computing $H^{-1}b$ directly, we will compute a Hessian vector product, which can be efficiently done by backprop through the model twice with $O(p)$ time complexity. The aforementioned conjugate gradient method requires the Hessian matrix to be positive definite. However, in practice the Hessian may have negative eigenvalues, since we run a SGD and the final H may not at a local minimum exactly. To tackle this issue, we solve $\arg \min_x \left\{ \frac{1}{2} x^T H^2 x - b^T H x \right\}$, whose solution can be shown the same as (15) since the Hessian matrix is symmetric. H^2 is guaranteed to be positive definite as long as H is not singular. The rate of convergence of the conjugate gradient depends on $\frac{\sqrt{\kappa(H^2)-1}}{\sqrt{\kappa(H^2)+1}}$, where $\kappa(H^2)$ is the condition number of H^2 , which can be very large if H is ill-conditioned. To encourage faster convergence, we add a small damping term λ on the diagonal and solve $\arg \min_x \left\{ \frac{1}{2} x^T (H^2 + \lambda I) x - b^T H x \right\}$.

Time Complexity As mentioned above, we can get an inverse Hessian vector product in $O(p)$ time. Since F and G are summation of loss with respect to all pretrain or finetune examples, it takes $O(mp)$ or $O(np)$ to compute Hessian vector product, where m is the number of pretrain examples and n is the number of finetune examples. We may subsample the pretrain examples to estimate $G(W, U)$ when the number of pretrain examples is gigantic such as pretrain using One-Billion-word dataset (Chelba et al., 2013) for ELMo etc. For the inverse Hessian vector product, the time complexity is $O(npr)$, where r is the number of iterations in CG.

4 EXPERIMENTS

In this section, we will conduct experiment with real datasets on both vision and NLP tasks to show the effectiveness of our proposed influence function. We will show the results in the main text on the vision tasks, and some qualitative results on NLP task related to ELMo are presented in Section C in Appendix.

4.1 INFLUENCE FUNCTION CORRELATION WITH REAL SCORE

To show that our proposed influence score are a good approximation, we evaluate our proposed multi-stage influence function on two CNN models with CIFAR and MNIST datasets. The model structures are shown in Table A in Appendix. We use Tanh for all activations. For both MNIST and CIFAR models, CNN layers are used as embeddings and fully connected layers are task-specific. At the pretrain stage, we train the models with examples from only two classes (“bird” vs. “frog”) for CIFAR and four classes (0, 1, 2, and 3) for MNIST. The resulting embedding is used in the finetune tasks, where we finetune the model with the examples from the remaining eight classes in CIFAR or the other 6 numbers in MNIST task for classification. In order to make the experiments closer to typical real finetune situations, we reduce the size of the training set in the finetune task by subsampling.

In this experiment we test the correlation between individual pretrain example’s multi-stage influence function and the real loss difference when the pretrain examples are removed. We test two cases (as mentioned in Section 3.1) – where the pretrain embedding is fixed, and where it is updated during finetune. For both MNIST and CIFAR, we first train the embedding with the binary classification for T_{pretrain} steps. The embedding is then used in the finetune model. Then we train the finetune model for T_{finetune} steps. Depending on different scenarios which will be explained below, the embedding may be fixed or updated in the finetune task training. For a given example in the pretrain data, we calculate its influence function score with respect to each test example in the finetune task test set using the method presented in Section 3. To evaluate this pretrain example’s contribution to the

overall performance of the model, we sum up the influence function scores across the whole test set in the finetune task.

To validate the score, we remove that pretrain example and go through the aforementioned process again by updating the model. In the updating process we further train the pretrain and finetune models for T'_{pretrain} and T'_{finetune} steps from the original model checkpoints. Note that in this process the pretrain is conducted with the new leave-one-out pretrain set, while the training set for the finetune task is intact. Due to computation constraints, we only use the top 100 pretrain examples with the largest influence function absolute values in this experiments to get 100 score-difference pairs. Then we run a linear regression between the true loss difference values obtained and the influence score computed to show their correlation. The detailed hyperparameters used in these experiments are presented in Appendix B.

4.1.1 EMBEDDING IS FIXED

In Figure 2 we show the correlation results of CIFAR and MNIST models when the embedding is fixed in finetune task training. Though we make many approximations in our formulation, from Figures 2a and 2b we can see that there is a clear linear approximations in our formulation and the influence function scores obtained. The correlation is evaluated with Pearson’s r value. This supports our argument that we can use this score to detect the examples in the pretrain set which contributes most to the model’s performance. In Figure 3 we demonstrate the misclassified test

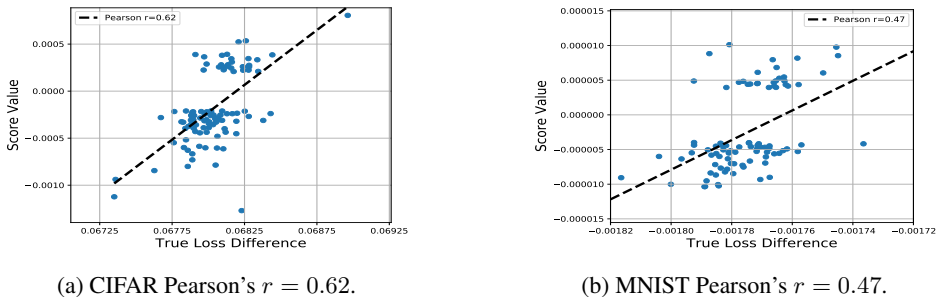


Figure 2: CIFAR and MNIST model true loss difference vs. the influence function scores by (8). The loss is calculated as the sum of all test examples.

images in the finetune task and the images with the largest positive influence function score in the pretrain dataset. Examples with large positive influence score are expected to have negative effect on the model’s performance since intuitively when they are added to the pretrain dataset, the loss of the test example will increase. From Figure 3 we can indeed see that the identified examples are with low quality, and they can be easily misclassified even with human eyes.

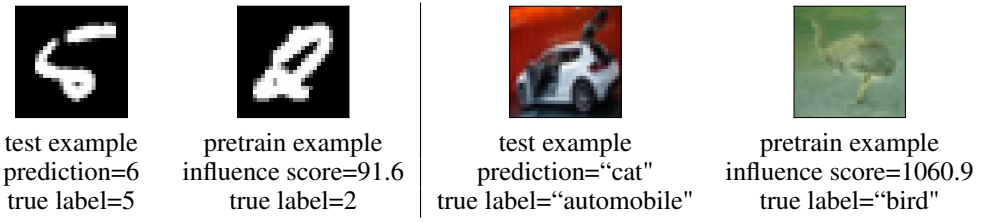


Figure 3: Identifying the pretrain example with largest influence function score which contributes an error in the finetune task.

One may doubt the effectiveness of the expensive inverse Hessian computation in our formulation. As a comparison, we replace all inverse Hessians in (11) with identity matrices to compute the influence function score for the MNIST model. The results are shown in Figure 4 with a much smaller Pearson’s r of 0.17. This again shows effectiveness of our proposed influence function.

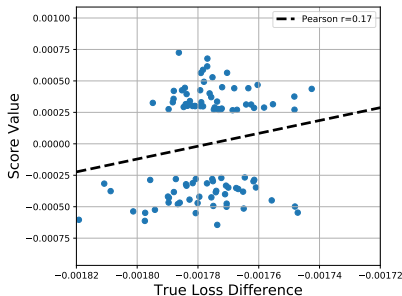


Figure 4: MNIST model true loss difference and influence function with all Hessians replaced by identity matrices. Pearson’s $r = 0.17$.

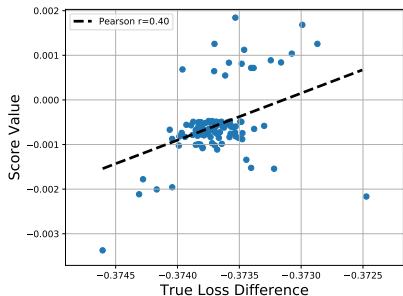


Figure 5: CIFAR example using ℓ_2 regularization formulation in (13) when embedding is not fixed in finetune. Pearson’s $r = 0.40$.

4.1.2 EMBEDDING IS UPDATED IN FINETUNE

Practically, the embedding can also be updated in the finetune process. In Figure 5 we show the correlation between true loss difference and influence function score values using (13). We can see that even under this challenging condition, our multi-stage influence function from (13) still has a strong correlation with the true loss difference, with a Pearson’s $r = 0.40$.

4.2 FINETUNE TASK SIMILARITY TO THE PRETRAIN TASK

In this experiment, we explore the relationship between influence function score and finetune task similarity with the pretrain task. Specifically, we study whether the influence function score will increase in absolute value if the finetune task is very similar to the pretrain task. To do this, we use the CIFAR embedding obtained from a “bird vs. frog” classification and test its influence function core on two finetune tasks. The finetune task A is exactly the same as the pretrain “bird vs. frog” classification, while the finetune task B is a classification on two other classes (“automobile vs. deer”). All hyperparameters used in the two finetune tasks are the same. In Figure 6, for both tasks we plot the distribution of the influence function values with respect to each pretrain example. We sum up the influence score for all test examples. We can see that, the first finetune task influence function has much larger absolute values than that of the second task. The average absolute value of task A influence function score is 0.055, much larger than that of task B, which is 0.025. This supports the argument that if pretrain task and finetune task are similar, the pretrain data will have larger influence on the finetune task performance.

4.3 INFLUENCE FUNCTION SCORE WITH DIFFERENT NUMBER OF FINETUNE EXAMPLES

We also study the relationship between the influence function scores and number of examples used in finetune. In this experiment, we update the pretrain embedding in finetune stage. We use the same pretrain and finetune task as in Section 4.1. In Figure 7, model C is the model used in Section 4.1.2 while in model D we triple the number of finetune examples as well as the number of finetune steps. Figure 7 demonstrates the distribution of each pretrain examples’ influence function score with the whole test set. The average absolute value of influence function score in model D is 0.15, much less than that of model C. This indicates that with more finetune examples and more finetune steps, the influence of pretrain data to the finetune model’s performance will decrease. This makes sense as if the finetune data does not have sufficient information for training a good finetune task, then pretrain data will have more impact on the finetune task.

5 CONCLUSION

We introduce a multi-stage influence function to evaluate pretrain examples’ contribution to finetune model’s prediction. Two different cases are studied: the pretrain embedding is fixed in finetune or the pretrain embedding is updated in finetune. We test our method on both CV and NLP tasks. Our experimental results show strong correlation between the proposed multi-stage influence function scores and the true loss difference when an example is removed from the pretrain data. We believe this is a promising way to connect finetune model’s performance with pretrain data directly.

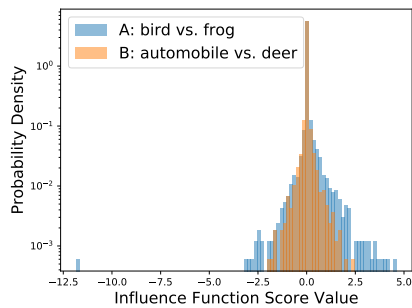


Figure 6: Two different finetunetask distribution of influence function scores with respect to each pretrain example. Each pretrain example’s influence score value is summed up for all test examples. The pre-trained embedding is fixed in finetune. For both finetune tasks, the pretrain model is the same, and is trained using “bird vs. frog” in CIFAR. For model A, finetune task and pretrain task are the same. The average absolute values of influence function scores for models A and B are 0.055 and 0.025, respectively.

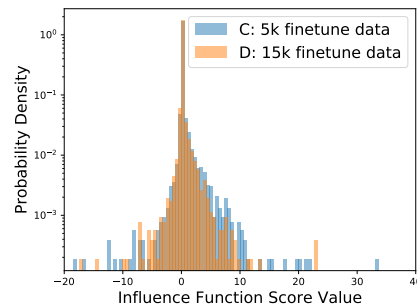


Figure 7: Two different finetune task distribution of influence function scores which respect to each pretrain example. Each pretrain example’s influence score value is summed up for all test examples. The pre-trained embedding is also updated in finetune. The pretrain and finetune tasks are the same as in Section 4.1.2. Model D’s number of finetune examples and finetune steps are 3X of model C’s. The average absolute values of influence function scores for Models C and D are 0.22 and 0.15, respectively.

REFERENCES

- Rie Kubota Ando and Tong Zhang. A framework for learning predictive structures from multiple tasks and unlabeled data. *J. Mach. Learn. Res.*, 6:1817–1853, 2005.
- Marc-Etienne Brunet, Colleen Alkalay-Houlihan, Ashton Anderson, and Richard Zemel. Understanding the origins of bias in word embeddings. In *ICML*, pp. 803–811, 2019.
- Ciprian Chelba, Tomas Mikolov, Mike Schuster, Qi Ge, Thorsten Brants, Phillipp Koehn, and Tony Robinson. One billion word benchmark for measuring progress in statistical language modeling. *arXiv preprint arXiv:1312.3005*, 2013.
- R. Dennis Cook and Sanford Weisberg. Characterizations of an empirical influence function for detecting influential cases in regression. *Technometrics*, 22(4):495–508, 1980.
- Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.
- Tian Guo, Tao Lin, and Nino Antulov-Fantulin. Exploring interpretable LSTM neural networks over multi-variable data. In *Proceedings of the 36th International Conference on Machine Learning*, pp. 2494–2504, 2019.
- K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In *2016 IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 770–778, 2016.
- Pang Wei Koh and Percy Liang. Understanding black-box predictions via influence functions. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pp. 1885–1894. JMLR. org, 2017.
- Pang Wei Koh, Kai-Siang Ang, Hubert H. K. Teo, and Percy Liang. On the accuracy of influence functions for measuring group effects. In *NeurIPS*, 2019.
- Hugo Larochelle, Dumitru Erhan, and Yoshua Bengio. Zero-data learning of new tasks. In *Proceedings of the 23rd National Conference on Artificial Intelligence - Volume 2, AAAI’08*, pp. 646–651, 2008.

- Dhruv Mahajan, Ross Girshick, Vignesh Ramanathan, Kaiming He, Manohar Paluri, Yixuan Li, Ashwin Bharambe, and Laurens van der Maaten. Exploring the limits of weakly supervised pretraining. In *Proceedings of the European Conference on Computer Vision (ECCV)*, pp. 181–196, 2018.
- Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems*, pp. 3111–3119, 2013.
- Jose Oramas, Kaili Wang, and Tinne Tuytelaars. Visual explanation by interpretation: Improving visual feedback capabilities of deep neural networks. In *International Conference on Learning Representations*, 2019.
- Jeffrey Pennington, Richard Socher, and Christopher Manning. Glove: Global vectors for word representation. In *Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP)*, pp. 1532–1543, 2014.
- Matthew E Peters, Mark Neumann, Mohit Iyyer, Matt Gardner, Christopher Clark, Kenton Lee, and Luke Zettlemoyer. Deep contextualized word representations. *arXiv preprint arXiv:1802.05365*, 2018.
- Jacob Steinhardt, Pang Wei Koh, and Percy Liang. Certified defenses for data poisoning attacks. In *Proceedings of the 31st International Conference on Neural Information Processing Systems*, pp. 3520–3532, 2017.
- Hao Wang, Berk Ustun, and Flávio P. Calmon. Repairing without retraining: Avoiding disparate impact with counterfactual distributions. In *Proceedings of the 36th International Conference on Machine Learning, ICML 2019, 9-15 June 2019, Long Beach, California, USA*, pp. 6618–6627, 2019.

A PROOF OF THEOREM 1

Proof. Since $\hat{\Theta}_\epsilon, \hat{U}_\epsilon, \hat{W}_\epsilon$ are optimal solutions, and thus satisfy the following optimality conditions:

$$0 = \frac{\partial}{\partial \Theta} F(\hat{W}_\epsilon, \hat{\Theta}_\epsilon) \quad (16)$$

$$0 = \frac{\partial}{\partial (W, U)} G(\hat{W}_\epsilon, \hat{U}_\epsilon) + \epsilon \frac{\partial}{\partial (W, U)} g(z, \hat{W}_\epsilon, \hat{U}_\epsilon), \quad (17)$$

where $\partial(W, U)$ means concatenate the U and W as $[W, U]$ and compute the gradient w.r.t $[W, U]$. We define the changes of parameters as $\Delta W_\epsilon = \hat{W}_\epsilon - \hat{W}$, $\Delta \Theta_\epsilon = \hat{\Theta}_\epsilon - \hat{\Theta}$, and $\Delta U_\epsilon = \hat{U}_\epsilon - \hat{U}$. Applying Taylor expansion to the rhs of (17) we get

$$0 \approx \frac{\partial}{\partial (W, U)} G(W^*, U^*) + \frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \begin{bmatrix} \Delta W_\epsilon \\ \Delta U_\epsilon \end{bmatrix} + \epsilon \frac{\partial g(z, W^*, U^*)}{\partial (W, U)} + \epsilon \frac{\partial^2 g(z, W^*, U^*)}{\partial (W, U)^2} \begin{bmatrix} \Delta W_\epsilon \\ \Delta U_\epsilon \end{bmatrix} \quad (18)$$

Since W^*, U^* are optimal of unperturbed problem, $\frac{\partial}{\partial (W, U)} G(W^*, U^*) = 0$, and we have

$$\begin{bmatrix} \Delta W_\epsilon \\ \Delta U_\epsilon \end{bmatrix} \approx - \left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} + \epsilon \frac{\partial^2 g(z, W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \epsilon \quad (19)$$

Since $\epsilon \rightarrow 0$, we have further approximation

$$\begin{bmatrix} \Delta W_\epsilon \\ \Delta U_\epsilon \end{bmatrix} \approx \left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \epsilon \quad (20)$$

Similarly, based on (16) and applying first order Taylor expansion to its rhs we have

$$0 \approx \frac{\partial F(W^*, \Theta^*)}{\partial \Theta} + \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} \cdot \Delta W_\epsilon + \frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} \Delta \Theta_\epsilon. \quad (21)$$

Combining (21) with (20) we have

$$\Delta \Theta_\epsilon \approx \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} \right)^{-1} \cdot \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} \right) \cdot \left[\left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \right]_W \epsilon$$

where $[\cdot]_W$ means taking the W part of the vector. Therefore,

$$I_{z, W} := \frac{\partial \hat{W}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} = - \left[\left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \right]_W \quad (22)$$

$$I_{z, \Theta} := \frac{\partial \hat{\Theta}_\epsilon}{\partial \epsilon} \Big|_{\epsilon=0} = \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta^2} \right)^{-1} \cdot \left(\frac{\partial^2 F(W^*, \Theta^*)}{\partial \Theta \partial W} \right) \cdot \left[\left(\frac{\partial^2 G(W^*, U^*)}{\partial (W, U)^2} \right)^{-1} \left(\frac{\partial g(z, W^*, U^*)}{\partial (W, U)} \right) \right]_W \quad (23)$$

□

B MODELS AND HYPERPARAMETERS FOR THE EXPERIMENTS IN SECTIONS 4.1, 4.2 AND 4.3

The model structures we used in Sections 4.1, 4.2 and 4.3 are listed in Table A. As mentioned in the main text, for all models, CNN layers are used as embeddings and fully connected layers are task-specific. The number of neurons on the last fully connected layer is determined by the number of classes in the classification. There is no activation at the final output layer and all other activations are Tanh.

- For MNIST experiments in Section 4.1.1, we train a four-class classification (0, 1, 2, and 3) in pretrain. All examples in the original MNIST training set with these four labels are used in pretrain. The finetune task is to classify the rest six classes, and we subsample only

5000 examples to finetune. The pretrained embedding is fixed in finetune. We run Adam optimizer to train both pretrain and fine tune model with a batch size of 512. The pretrain and finetune models are trained to converge. When validating the influence function score, we remove an example from pretrain dataset. Then we re-run the pretrain and finetune process with this leave-one-out pretrain dataset starting from the original models’ weights. In this process, we only run 100 steps for pretrain and finetune as the models converge. When computing the influence function scores, the damping term for the pretrain and finetune model’s Hessians are 1×10^{-2} and 1×10^{-8} , respectively. We sample 1000 pretrain examples when computing the pretrain model’s Hessian summation.

- For CIFAR experiments in Section 4.1.1, we train a two-class classification (“bird” vs “frog”) in pretrain. All examples in the original CIFAR training set with these four labels are used in pretrain. The finetune task is to classify the rest eight classes, and we subsample only 5000 examples to finetune. The pretrained embedding is fixed in finetune. We run Adam optimizer to train both pretrain and fine tune model with a batch size of 128. The pretrain and finetune models are trained to converge. When validating the influence function score, we remove an example from pretrain dataset. Then we re-run the pretrain and finetune process with this leave-one-out pretrain dataset starting from the original models’ weights. In this process, we only run 6000 steps for pretrain and 3000 steps for finetune. When computing the influence function scores, the damping term for the pretrain and finetune model’s Hessians are 1×10^{-8} and 1×10^{-6} , respectively. Same hyperparameters are used in experiments in Sections 4.2 and 4.3. We also use these hyperparameters in Section 4.1.2’s experiments, except that the pretrained embedding is updated in finetune and the number of finetune steps is reduced to 1000 in validation. The α constant in Equation 14 is chosen as 0.01. We sample 1000 pretrain examples when computing the pretrain model’s Hessian summation.

Dataset	MNIST	CIFAR
Embedding	CONV 32 $5 \times 5 + 1$	CONV 32 $3 \times 3 + 1$
	MAX-POOL $2 \times 2 + 2$	CONV 64 $4 \times 4 + 1$
	CONV 64 $5 \times 5 + 1$	MAX-POOL $2 \times 2 + 2$
	MAX-POOL $2 \times 2 + 2$	CONV 128 $2 \times 2 + 1$
		MAX-POOL $2 \times 2 + 2$
		CONV 128 $2 \times 2 + 1$
		MAX-POOL $2 \times 2 + 2$
Task specific	FC <# classes>	FC 1500 FC <# classes>

Table A: Model Architectures. “CONV $k \ w \times h + s$ ” represents a 2D convolutional layer with k filters of size $w \times h$ using a stride of s in both dimensions. “MAX-POOL $w \times h + s$ ” represents a 2D max pooling layer with kernel size $w \times h$ using a stride of s in both dimensions. “FC n ” = fully connected layer with n outputs. All activation functions are Tanh and last fully connected layers do not have activation functions. The number of neurons on the last fully connected layer is determined by the number of classes in the task.

C ELMO EXPERIMENT

In this section we show influence function score results with ELMO. The finetune task is a binary sentiment classification of twitter¹ and the ELMO model is pretrained on a one-billion-word dataset Chelba et al. (2013). For the finetune model, we add a hidden layer with 64 neurons and an output layer to build the classifier. The activation function is Tanh. For simplicity, we use the original pretrained ELMO embedding and the embedding is fixed in finetune. We randomly sample a subset of 1000 sentences from one-billion-word dataset. For a test sentence, we list the pretrain sentences with the largest and the smallest absolute influence function score values in one-billion-word dataset.

¹ https://datahack.analyticsvidhya.com/contest/linguipedia-codefest-natural-language-processing-1/#data_dictionary

Test Sentence	Max abs. score	Sentence in Pretrain	Min abs. score	Sentence in Pretrain
<i>Finally a transparent silicon case Thanks to my uncle :) #yay #Sony #Xperia #S #sonyexperias...</i>	-0.0049	<i>Prof Slobodchikoff details the experiments he has done to reveal the hidden structure of the prairie dog 's language within the BBC natural history programme " Prairie dogs , talk of the town , " broadcast as part of the Natural World documentary series .</i>	6.74×10^{-9}	<i>He will be there to help you . "</i>
<i>Bout to go shopping again listening to music #iphone #justme #music #likeforlike #followforfollow...</i>	0.0014	<i>We are seeing the first big systematic investment in dance .</i>	-6.30×10^{-9}	<i>The war seemed to energize her , and she began to hang out with the American journalists based in London .</i>
<i>Ha! Not heavy machinery but it does what I need it to. @Apple really dropped the ball with that design. #drinkyourhaterade</i>	0.00052	<i>He 's been on the move since his comeback victory over Juan Manuel Marquez more than two weeks ago , a brutally efficient boxing display that generated a staggering 1 million pay-per-view buys .</i>	-2.25×10^{-9}	<i>Taylor said the syndicated TV psychologist broached the idea of the show to Spears ' handlers , who eventually decided that such a show would be " detrimental " to the family .</i>

Table B: The list of test sentences and pretrain sentences with the largest and the smallest absolute influence function score values in our subset of pretrain data. The subset consists of 1000 random sentences from one-billion-word, which is used to pretrain ELMo embedding.